While calculating RKKY interaction in graphene no theorist should do a cut-off without cause

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In our previous work (E. Kogan, Phys. Rev. B **84**, 115119 (2011)) we presented calculation of RKKY interaction between two magnetic impurities in graphene based on Matsubara Green's functions (MGF) in the coordinate – imaginary time representation. Now we present the calculation based on MGF in the coordinate – frequency representation. We claim that both approaches have an important advantage over those based on zero temperature Green's functions (ZTGF), which are very briefly reviewed in the beginning of the present work. The MGF approaches, in distinction to the ZTGF approaches, operate only with the convergent integrals from the start to the end of the calculation. The coordinate – frequency representation for the MGF turns out to be as convenient as the coordinate – imaginary time representation and allows to easily consider the cases of doped and gapped graphene.

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INTRODUCTION

RKKY interaction between two magnetic impurities in graphene was theoretically studied quite intensely during last several years [1–18]. (A terse but precise review of the issue one can find in the book by M. Katsnelson [19].) One may ask, why the problem, which is in principle so simple (when being treated in the lowest order of perturbation theory, like it was done in all the papers referenced above), was the subject of so many publication, using different approaches? The answer to this question, as presented below, is connected with the fact that a simply written integral is not necessarily a simply calculated integral, and in the frame work of all zero temperature Green's functions (ZTGF) the integrals defining the RKKY interaction in graphene turned out to be divergent. Different ZTGF approaches can be thus viewed as different ways to obtain finite results from the divergent integrals.

In our previous publication dealing with the subject we were using the approach based on Matsubara Green's functions (MGF) in the coordinate – imaginary time representation [11]. In this work we consider RKKY interaction in graphene in the framework of approach based on MGF in the coordinate – frequency representation, and find that this approach is no less convenient than the one we used previously. Before we present the approach, we give a brief review of the existing ZTGF approaches, indicating explicitly where the divergent integrals appear.

If we ignore the spin–orbit coupling, the effective exchange RKKY interaction between the two magnetic impurities with the spins $\mathbf{S}_1$ and $\mathbf{S}_2$, sitting on top of carbon atoms at the sites i and j, is

$$H_{RKKY} = -\frac{1}{4}J^2\chi(i,j)\mathbf{S}_1\cdot\mathbf{S}_2, \tag{1}$$

where J is the contact exchange interaction between each of spins and the graphene electrons, and χ_R is the free electrons charge susceptibility. Thus different approached to calculation of the RKKY interaction are actually different approaches to calculation the susceptibility.

Not to distract attention of the reader from the aspects of the physics we are going to concentrate upon, we'll consider a toy model of graphene, with free electrons being described by the 2d Dirac Hamiltonian. Thus the model can possess only a single Dirac point, and we'll present the existing approaches as if they were applied to this toy model. Notice, that due to the isotropy of the model

$$\chi(i,j) = \chi(R), \tag{2}$$

where R is the distance between the sites i and j.

APPROACHES BASED ON ZTGF

The approach, used in Refs. [1, 3, 4] is based on equation

$$\chi(R) = \int \frac{d^2\mathbf{q}}{(2\pi)^2}\chi(\omega=0,\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{R}}, \tag{3}$$

where

$$\chi(\omega=0,\mathbf{q}) = 2\int \frac{d^2\mathbf{k}}{(2\pi)^2}\frac{n_F(\xi_{\mathbf{k}}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})}{E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}}}; \tag{4}$$

$\xi_n = E_n - \mu$ and $n_F(\xi) = \left(e^{\beta\xi}+1\right)^{-1}$ is the Fermi distribution function. This approach, though looking quite straightforward, brings with it a problem. In a model of infinite Dirac cones for $\chi(\omega=0,\mathbf{q})$ we obtain a diverging integral. To obtain finite values from these divergent integrals, as it was mentioned previously, one has to implement the complicated (and to some extent arbitrary) cut-off procedure [4].

The problem can be formulated in a different way. Being calculated in a realistic band model, with the bands

of finite width, $\chi(\omega=0,\mathbf{q})$ is not a universal quantity. It depends not only on infrared physics, but on the properties of electron spectrum and eigenfunctions in the whole Brillouin zone (even for small $\mathbf{q}$).

Another approach, formulated in Ref. [2], starts from a well known equation for the susceptibility

$$\chi(R)=\frac{2i}{\pi}\int_{-\infty}^{\infty}G^2(R,E)dE, \tag{5}$$

where G is the retarded green's function. Here again the integral diverges on both limits of integration. However the authors changed the contour of integration, transforming the divergent integral (5) into the convergent integral along the imaginary axis (see also Ref. [20]). The authors also considered RKKY interaction in gapped graphene, when the power law decrease of the interaction with the distance turns into the exponential law. Actually, in a implicit form the authors made the transition from ZTGF to MGF, so our final results will be very close to ones obtained in Ref. [2].

The approach, using formula

$$\chi(r,r')=\delta n(r)/\delta V(r') \tag{6}$$

and, hence, calculating electron susceptibility on the basis of equation

$$\chi(R)=-\frac{2}{\pi}\int_{-\infty}^{E_F}\mathrm{Im}\left[G^2(R,E)\right]dE, \tag{7}$$

where E_F is the Fermi energy, was first used, in application to graphene to the best of our knowledge, in Ref. [7]. An advantage of this approach is that it allows to easily consider the case of doped graphene, the disadvantage is that the approach, like the one presented above, has to deal with the divergent integral (the integral with respect to dE diverges at the lower limit of integration). Also in this case, to obtain finite values from these divergent integrals one has to implement the complicated (and to some extent arbitrary) cut-off procedure.

MGF IN FREQUENCY REPRESENTATION

Our approach will be based on equation [21]

$$\chi(R)=-\frac{1}{\pi}\int_{-\infty}^{\infty}\mathcal{G}^2(R;\omega)d\omega, \tag{8}$$

where $\mathcal{G}(R;\omega)$ is the MGF in frequency momentum representation. Dirac equation describing electrons is

$$H=v(\tau^x k_x+\tau^y k_y), \tag{9}$$

where the matrix τ acts in the space of two sublattices. From Eq. (9) we obtain

$$\mathcal{G}(k,\omega)=\frac{1}{i\omega+\mu-v(\tau^x k_x+\tau^y k_y)}, \tag{10}$$

where μ is a chemical potential. From Eq. (10) we obtain [22]

$$\mathcal{G}^{CC}(R,\omega)=\frac{-i(\omega-i\mu)}{(2\pi)^2}\int_0^{\infty}\frac{kdk}{(\omega-i\mu)^2+v^2k^2}$$
$$\cdot\int_0^{2\pi}e^{ikR\cos\theta}d\theta=\frac{-i(\omega-i\mu)}{2\pi}\int_0^{\infty}\frac{kJ_0(kR)dk}{(\omega-i\mu)^2+v^2k^2}$$
$$=\frac{-i(\omega-i\mu)}{2\pi v^2}K_0\left[\mathrm{sign}(\omega)(\omega-i\mu)R/v\right]. \tag{11}$$

$$\mathcal{G}^{AB}(R,\omega)=\frac{-v}{(2\pi)^2}\int_0^{\infty}\frac{k^2dk}{(\omega-i\mu)^2+v^2k^2}$$
$$\cdot\int_0^{2\pi}e^{ikR\cos\theta+i\theta}d\theta=\frac{-v}{2\pi}\int_0^{\infty}\frac{k^2J_1(kR)dk}{(\omega-i\mu)^2+v^2k^2}$$
$$=\frac{-\mathrm{sign}(\omega)(\omega-i\mu)}{2\pi v^2}K_1\left[\mathrm{sign}(\omega)(\omega-i\mu)R/v\right]. \tag{12}$$

(CC can mean either AA or BB; K_0 and K_1 are the modified Bessel function of zero and first order respectively). We have used mathematical identity, valid for Re $z>0$ [23],

$$\int_0^{\infty}\frac{x^{\nu+1}}{(x^2+z^2)^{\rho}}J_{\nu}(cx)dx=\frac{c^{\rho-1}z^{\nu-\rho+1}}{2^{\rho-1}\Gamma(\rho)}K_{\nu-\rho+1}(cz). \tag{13}$$

UNDOPED GRAPHENE

Consider first the case of undoped graphene ($\mu=0$).

MGF in frequency representation

Using another mathematical identity [23]

$$\int_0^{\infty}x^{\alpha-1}K_{\mu}(cx)K_{\nu}(cx)dx=\frac{2^{\alpha-3}}{c^{\alpha}\Gamma(\alpha)}\Gamma\left(\frac{\alpha+\mu+\nu}{2}\right)$$
$$\Gamma\left(\frac{\alpha+\mu-\nu}{2}\right)\Gamma\left(\frac{\alpha-\mu+\nu}{2}\right)\Gamma\left(\frac{\alpha-\mu-\nu}{2}\right), \tag{14}$$

from Eq. (8) we obtain [4]

$$\chi^{AA}_{\mu=0}(R)=\frac{1}{64\pi vR^3},\qquad \chi^{AB}_{\mu=0}(R)=-\frac{3}{64\pi vR^3}. \tag{15}$$

MGF in time representation

For completeness, we reproduce here the calculation of χ based on MGF in coordinate – imaginary time representation, presented in our previous paper [11]. The susceptibility was written as [4, 5, 11]

$$\chi(R)=-2\int_{-\infty}^{\infty}\mathcal{G}(R;\tau)\mathcal{G}(R;-\tau)d\tau. \tag{16}$$

Transition from frequency to imaginary time representation yields the MGF

$$\mathcal{G}^{CC}(\mathbf{k},\tau) = \frac{\mathrm{sign}(\tau)}{2} e^{-vk|\tau|}$$
$$\mathcal{G}^{AB}(\mathbf{k},\tau) = \frac{1}{2} e^{-vk|\tau|+i\theta}. \quad (17)$$

As a result we obtain [11]

$$\mathcal{G}^{CC}(R,\tau) = \frac{\mathrm{sign}(\tau)}{8\pi^2}\int_0^\infty dkk\int_0^{2\pi} d\theta e^{ikR\cos\theta - vk|\tau|}$$
$$\mathcal{G}^{AB}(R,\tau) = \frac{1}{8\pi^2}\int_0^\infty dkk\int_0^{2\pi} d\theta e^{ikR\cos\theta + i\theta - vk|\tau|}. \quad (18)$$

Performing the angular integrations in Eq. (18) we get

$$\mathcal{G}^{CC}(R;\tau) = \frac{\mathrm{sign}(\tau)}{4\pi}\int_0^\infty dkkJ_0(kR)e^{-vk|\tau|}$$
$$\mathcal{G}^{AB}(R;\tau) = \frac{1}{4\pi}\int_0^\infty dkkJ_1(kR)e^{-vk|\tau|}. \quad (19)$$

(J_0 and J_1 are the Bessel function of zero and first order respectively). Using mathematical identity [23]

$$\int_0^\infty x^{n-1}e^{-px}J_\nu(cx)dx \quad (20)$$
$$= (-1)^{n-1}c^{-\nu}\frac{\partial^{n-1}}{\partial p^{n-1}}\frac{\left(\sqrt{p^2+c^2}-p\right)^\nu}{\sqrt{p^2+c^2}},$$

integrals in the RHS of Eq. (19) can be calculated exactly, giving a well known result [5]

$$\mathcal{G}^{CC}(R;\tau) = \frac{1}{4\pi}\frac{v\tau}{(v^2\tau^2+R^2)^{3/2}}$$
$$\mathcal{G}^{AB}(R;\tau) = \frac{1}{4\pi}\frac{R}{(v^2\tau^2+R^2)^{3/2}}. \quad (21)$$

The remaining integration in Eq. (16) is trivial; as a result we recover Eq. (15).

DOPED GRAPHENE

In the case of doped graphene the susceptibility (8) will be expressed through the integrals

$$\mathrm{Re}\left\{\int_0^\infty (\omega-i\mu)^2 K_{0,1}^2\left[(\omega-i\mu)R/v\right]d\omega\right\}. \quad (22)$$

Considering integrals in the complex plane it is convenient to deform the contour of integration and present the integrals as

$$\mathrm{Re}\left\{\int_0^\infty \omega^2 K_{0,1}^2(\omega R/v)d\omega + \int_{-i\mu}^0 \omega^2 K_{0,1}^2(\omega R/v)d\omega\right\}. \quad (23)$$

Taking into account the identity

$$K_\alpha(-ix) = \frac{\pi}{2}i^{\alpha+1}[J_\alpha(x)+iY_\alpha(x)], \quad (24)$$

we get [12]

$$\chi_\mu^{CC}(R) = \chi_{\mu=0}^{CC}(R)\left[1-16\int_0^{k_FR} dzz^2J_0(z)Y_0(z)\right]$$
$$\chi_\mu^{AB}(R) = \chi_{\mu=0}^{AB}(R)\left[1+\frac{16}{3}\int_0^{k_FR} dzz^2J_1(z)Y_1(z)\right], \quad (25)$$

where $k_F = \mu/v$. The integrals in Eq. (25) can be presented in terms of Meijer functions [12] (I send the reader to that Reference for the details).

It is interesting to compare the RKKY exchange in doped graphene, with its two sublattices and linear dispersion law, with that in ordinary two-dimensional electron gas. For the latter the Green's function is

$$\mathcal{G}(k,\omega) = \frac{1}{i\omega+\mu-k^2/2m}. \quad (26)$$

Hence the susceptibility turns out to be [24]

$$\chi(R) \sim \frac{1}{R^2}\int_0^{k_FR} dzzJ_0(z)Y_0(z). \quad (27)$$

Amusing, that the authors of Ref. [24] were affiliated with the same University, as the author of the present paper.

GAPPED GRAPHENE

Consider now graphene with the gap in electron spectrum described by Dirac Hamiltonian

$$H = v(\tau^x k_x + \tau^y k_y) + \Delta\tau^z. \quad (28)$$

The Green's function is

$$\mathcal{G}(\mathbf{k},\omega) = \frac{-i\omega - \Delta\tau^z - v(\tau^x k_x+\tau^y k_y)}{\omega^2+\Delta^2+v^2k^2}. \quad (29)$$

MGF in frequency representation

From Eq. (29) we obtain

$$\mathcal{G}^{CC}(R,\omega) = \frac{-i\omega\mp\Delta}{2\pi}\int_0^\infty \frac{kJ_0(kR)dk}{\omega^2+\Delta^2+v^2k^2}$$
$$= \frac{-i\omega\pm\Delta}{2\pi v^2}K_0\left(\sqrt{\omega^2+\Delta^2}R/v\right). \quad (30)$$

$$\mathcal{G}^{AB}(R,\omega) = \frac{-v}{2\pi}\int_0^\infty \frac{k^2J_1(kR)dk}{\omega^2+\Delta^2+v^2k^2}$$
$$= \frac{-\sqrt{\omega^2+\Delta^2}}{2\pi v^2}K_1\left(\sqrt{\omega^2+\Delta^2}R/v\right). \quad (31)$$

In Eq. (30) minus corresponds to AA and plus to BB. Substituting into Eq. (8) we obtain [25]

$$\chi^{CC}(R) = \frac{1}{4\pi^3 v^4} \int_{-\infty}^{\infty} (\omega^2 - \Delta^2) K_0^2 \left(\sqrt{\omega^2 + \Delta^2} R/v\right) d\omega. \quad (32)$$

$$\chi^{AB}(R) = -\frac{1}{4\pi^3 v^4} \int_{-\infty}^{\infty} (\omega^2 + \Delta^2) K_1^2 \left(\sqrt{\omega^2 + \Delta^2} R/v\right) d\omega. \quad (33)$$

The remaining integrations can be performed analytically in two limiting cases.

Consider first the case $\Delta R/v \ll 1$. Here it is appropriate to mention the relation between the toy model, we are using, and real graphene. The existence of two Dirac points in graphene leads to additional angular dependent factor in the formula for the RKKY interaction. It was thoroughly studied previously and does not interfere with the physics we are discussing in this work. More interesting is the condition of the applicability of the infinite Dirac cones dispersion law to the calculation of RKKY interaction in graphene. From Eq. (21) we see that characteristic values of τ entering into integral (16) are of the order of R/v; hence characteristic k entering into integrals (19) are of the order of $1/R$. Thus the approximation of linear dispersion law is applicable, provided $R \gg a$, where a is the graphene lattice constant. Now we realize, that the case $\Delta R/v \ll 1$ can be described in the framework of the model if $\Delta \ll av$, or in simple terms, if the gap is narrow in comparison with the graphene band width, which is certainly true in most cases of gapped graphene. So finally, in the case of a narrow gap and relatively small distances we can go to the limit $\Delta \to 0$ in Eqs. (32) and (33), and recover the results of the gapless case.

The other limiting case $\Delta R/v \gg 1$ is more interesting. In this case we may use asymptotic expression for modified Bessel functions

$$K_\nu(z) \sim \sqrt{\frac{\pi}{2z}} e^{-z}. \quad (34)$$

After calculating the resulting integrals in Eq. (33) using the Laplace method, we obtain the same result both for inter-sublattice and intra-sublattice susceptibility

$$\chi = -\frac{1}{8v} \left(\frac{\Delta}{\pi v R}\right)^{3/2} e^{-2R\Delta/v}. \quad (35)$$

It is worth paying attention to the fact that Eq. (35) seems to contradict rigorously proved theorem stating that for any bipartite lattice at half filling, the RKKY interaction is antiferromagnetic between impurities sitting on top of atoms belonging to opposite sublattices (i.e., A and B sublattices in graphene), and is ferromagnetic between impurities sitting on top of atoms belonging to the same sublattice [4, 11, 26]. However, the theorem is not applicable to Hamiltonian (28), with its last term meaning that if we rewrite the Hamiltonian in the tight-binding representation, the intra-sublattice hopping will appear, hence the lattice is no longer bipartite. More specifically, the spectrum still has the symmetry of that in bipartite lattice, but the wave functions do not [11].

MGF in time representation

Here we'll restrict ourselves with the calculation of χ^{AB}. Transition from frequency to imaginary time representation yields the MGF

$$\mathcal{G}^{AB}(\mathbf{k}, \tau) = \frac{1}{2} \frac{vk}{\sqrt{\Delta^2 + v^2 k^2}} e^{-\sqrt{\Delta^2 + v^2 k^2}|\tau| + i\theta}. \quad (36)$$

Hence instead of Eq. (19) we obtain

$$J_0(kR) e^{-\sqrt{\Delta^2 + v^2 k^2}|\tau|} \quad (37)$$

$$\mathcal{G}^{AB}(R; \tau) = \frac{v}{4\pi} \int_0^\infty dk \frac{k^2}{\sqrt{\Delta^2 + v^2 k^2}} J_1(kR) e^{-\sqrt{\Delta^2 + v^2 k^2}|\tau|}. \quad (38)$$

Using mathematical identity [23]

$$\int_0^\infty x^{\nu+1} \frac{e^{-p\sqrt{x^2+z^2}}}{\sqrt{x^2+z^2}} J_\nu(cx) dx = B_\nu, \quad (39)$$

where

$$B_1 = c \left(1 + z\sqrt{p^2 + c^2}\right) \frac{e^{-z\sqrt{p^2+c^2}}}{(p^2+c^2)^{3/2}},$$

we obtain

$$\mathcal{G}^{AB}(R; \tau) = \frac{R}{4\pi} \left(1 + \sqrt{v^2\tau^2 + R^2}\Delta/v\right) \frac{e^{-\sqrt{v^2\tau^2+R^2}\Delta/v}}{(v^2\tau^2 + R^2)^{3/2}}. \quad (40)$$

Thus we obtain

$$\chi^{AB}(R) = -\frac{R^2}{8\pi^2} \int_{-\infty}^{\infty} \left(1 + \sqrt{v^2\tau^2 + R^2}\Delta/v\right)^2 \frac{e^{-2\sqrt{v^2\tau^2+R^2}\Delta/v}}{(v^2\tau^2 + R^2)^3} d\tau. \quad (41)$$

In the case $\Delta R/v \gg 1$ we can calculate integral in Eq. (41) using the Laplace method, to recover Eq. (35).

CONCLUSIONS

In the end we would like to mention again that though we were considering the case of $T = 0$, we have found, that, as it is not infrequently happens, the MGF have advantages over ZTGF. In particular, using the former one have to operate only with the convergent integrals, in distinction to what happens when one uses the latter.

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[1] M. A. H. Vozmediano, M. P. Lopez-Sancho, T. Stauber and F. Guinea, Phys. Rev. B **72**, 155121 (2005).

[2] V. K. Dugaev, V. I. Litvinov and J. Barnas, Phys. Rev. B **74**, 224438 (2006).

[3] L. Brey, H. A. Fertig and S. D. Sarma, Phys. Rev. Let. **99**, 116802 (2007).

[4] S. Saremi, Phys. Rev. B **76**, 184430 (2007).

[5] V. V. Cheianov, O. Syljuasen, B. L. Altshuler, and V. Fal'ko, Phys. Rev. B **80**, 233409 (2009).

[6] A. M. Black–Schaffer, Phys. Rev. B **81**, 205416 (2010).

[7] M. Sherafati and S. Satpathy, Phys. Rev. B **83**, 165425 (2011).

[8] B. Uchoa, T. G. Rappoport, and A. H. Castro Neto, Phys. Rev. Lett. **106**, 016801 (2011).

[9] J. E. Bunder and H.-H. Lin, Phys. Rev. B **80**, 153414 (2009).

[10] S. R. Power and M. S. Ferreira, Phys. Rev. B **83**, 155432 (2011).

[11] E. Kogan, Phys. Rev. B **84**, 115119 (2011).

[12] M. Sherafati and S. Satpathy, Phys. Rev. B **84**, 125416 (2011).

[13] K. Szalowski Phys. Rev. B **84**, 205409 (2011).

[14] J. E. Bunder and James M. Hill, J. of Chem Phys **136**, 154504 (2012).

[15] H. Lee, J. Kim, E. R. Mucciolo, G. Bouzerar, S. Kettemann, Phys. Rev. B 85, 075420 (2012).

[16] M. Sherafati and S. Satpathy, AIP Conf. Proc. 1461, pp. 24-33; doi:http://dx.doi.org/10.1063/1.4736868.

[17] L. Jiang, X. Lu, W. Gao, G. Yu, Z. Liu, and Y. Zheng, J. Phys.: Condens. Matter **24**, 206003 (2012).

[18] J. Klinovaja and D. Loss, arXiv:1211.3067v1.

[19] M. I. Katsnelson, *Graphene: carbon in two dimensions*. Cambridge University Press (2012).

[20] V. I. Litvinov and V. K. Dugaev, Phys. Rev. B **58**, 3584 (1998).

[21] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyloshinski, *Methods of Quantum Field Theory in Statistical Physics*, (Pergamon Press, 1965).

[22] A.D. Shytov, D. A. Abanin, and L. S. Levitov, Phys. Rev. Lett. **103**, 016806 (2009).

[23] A. P. Prudnikov, Yu. A. Brychkov and O. I. Marichev, *Integrals and Series* Vol. 2 (Gordon and Breach Science Publishers, 1986).

[24] B. Fischer and M. W. Klein, Phys. Rev. B **11**, 2025 (1975).

[25] V. K. Dugaev, V. I. Litvinov and P. P. Petrov, Superlattices and Microstructures **16**, 413 (1994).

[26] V. M. Pereira, J. M. B. Lopes dos Santos, and A. H. Castro Neto, Phys. Rev. B **77**, 115109 (2008).